

4. (Once Amended) A computer-aided method for designing molecules according to claim

[3]1 wherein it further comprises the step:

screening the candidate molecules on the basis of enrichment in molecular diversity terms provided by each molecule in relation to the selected descriptors.

5. (Once Amended) A computer-aided method according to claim [3]1, wherein at least one of said criteria is based on a non-linear function of a descriptor value.

8. (Once Amended) A computer-aided method according to claim [3]2, wherein at least one of said dynamic criteria is based on the conformational spaces of a candidate molecule.

9. (Once Amended) A computer-aided method according to claim [3]2, wherein at least one of said dynamic criteria is based on a shape descriptor derived from a 3D autocorrelation vector (3D-ACV) of the candidate molecule.

10. (Once Amended) A computer-aided method according to claim [3]2, wherein the static criteria are based on physicochemical and topological descriptors at least some of which are chosen from the descriptors cited in Table II.

12. (Once Amended) A computer-aided method for the provision, identification and description of molecules exhibiting antibacterial activity, employing a step of molecular modelling a molecule having antibacterial activity, a step of building a combinatorial library including molecules having said antibacterial activity and a step of selecting potentially antibacterial molecules, wherein said method includes a step whereby the candidate molecules are filtered using a static filter representing a plurality of descriptors [or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said antibacterial activity].

15. (Once Amended) A computer-aided method for the provision, identification and description of molecules exhibiting antibiotic activity, employing a step of molecular modelling a molecule having antibiotic activity, a step of building a combinatorial library including molecules having said antibiotic activity and a step of selecting potentially antibiotic molecules, wherein said method includes a step whereby the candidate molecules are filtered using a static filter representing a plurality of descriptors [or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said antibiotic activity].

16. (Once Amended) A computer-aided method for the provision, identification and description of molecules exhibiting anti-viral activity, employing a step of molecular modelling a molecule having anti-viral activity, a step of building a combinatorial library including molecules having said anti-viral activity and a step of selecting potentially anti-viral molecules, wherein said method includes a step whereby the candidate molecules are filtered using a static filter representing a plurality of descriptors[or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said anti-viral activity].

17. (Once Amended) A computer-aided method for the provision, identification and description of molecules exhibiting anti-parasitic activity, employing a step of molecular modelling a molecule having anti-parasitic activity, a step of building a combinatorial library including molecules having said anti-parasitic activity and a step of selecting potentially anti-parasitic molecules, wherein said method includes a step whereby the candidate molecules are filtered using a static filter representing a plurality of descriptors[or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said anti-parasitic activity].

18. (Once Amended) A computer-aided method for the provision, identification and description of molecules exhibiting immunomodulatory, employing a step of molecular modelling a molecule having immunomodulatory activity, a step of building a combinatorial library including molecules having said immunomodulatory activity and a step of selecting potentially immunomodulatory molecules, wherein said method includes a step whereby the candidate molecules are filtered [or] using a static filter representing a plurality of descriptors[or using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said immunomodulatory activity].

Add new claims 65-72 as follows:

65. (New) A method according to claim 12 including the further step of using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said antibacterial activity.

66. (New) A method according to claim 15 including the further step of using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said antibiotic activity.